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Title:	How does Ga doping of -Pu affect the phonons?
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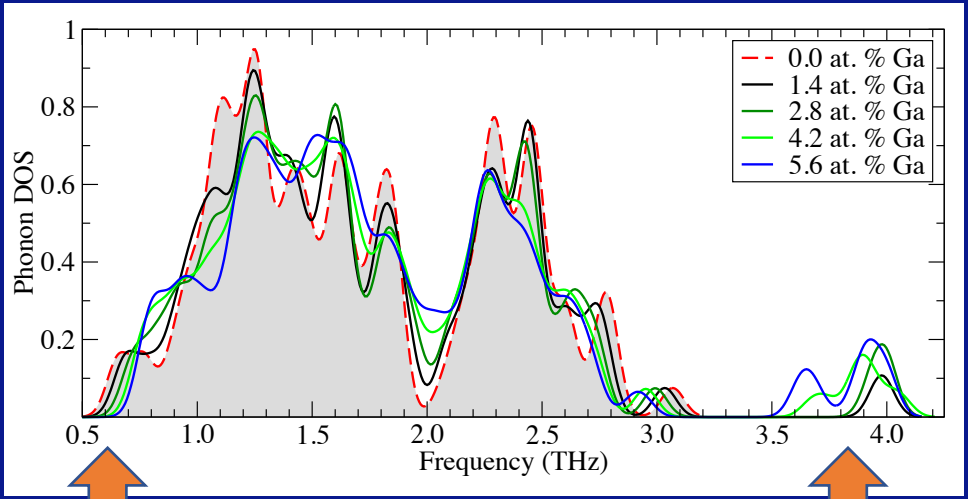
How does Ga doping of δ-Pu affect the phonons?



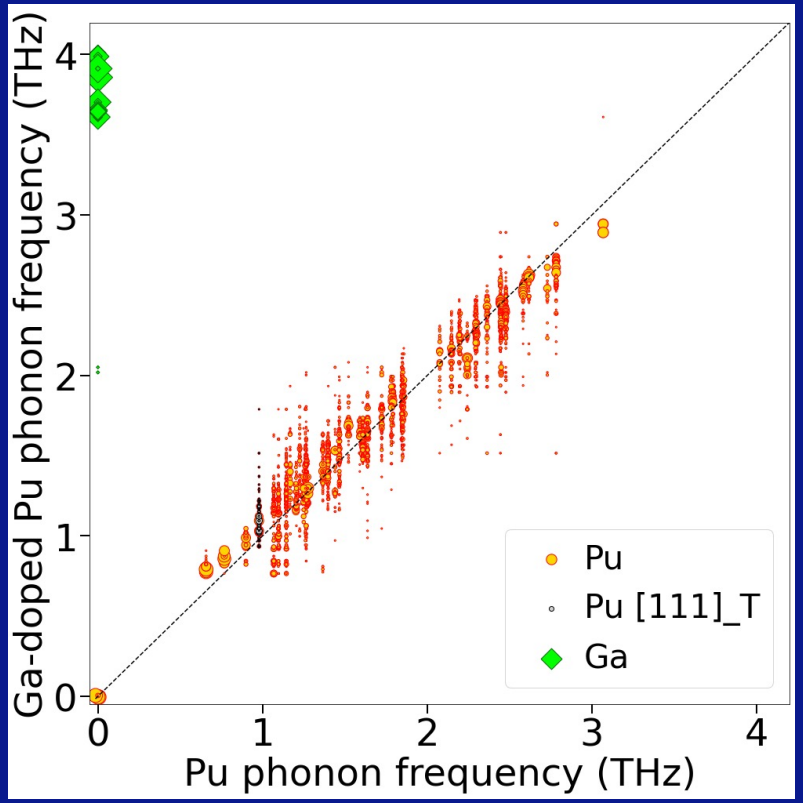
Ga doping stiffens low-frequency phonon modes.

Ga doping introduces high-frequency phonon modes.

As part of the LDRD-DR project "Aging and Metastability of Delta-Phase Plutonium," large-scale density functional theory calculations were performed to reveal details of how Ga doping affects the phonons of delta-phase Pu.

Phonons are where most of the heat is stored: these results improve our understanding of how Ga doping affects the thermal response of δ-Pu.

How does Ga doping of δ-Pu affect the phonons?



The low-frequency modes that become stiffer with Ga doping include the *T[111]* modes. These modes have been proposed to describe pathways for the transformation from the delta phase into the alpha phase.

This results in a plausible conclusion for how Ga doping stabilizes the delta phase: stiffening the *T[111]* modes makes it harder for the material to follow the delta-to-alpha transformation.